Quasi-random spatially balanced sampling

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Introduction

- Choosing an appropriate sampling design for a particular study can be difficult and there is no *best* design for all research questions.

- This choice depends on many things including the study objectives, available sampling frames and known auxiliary variables.

- This presentation focuses on estimating the population total of a response y using the unbiased Horvitz-Thompson estimator (or its continuous analogue)

$$\widehat{\tau} = \sum_{i \in \mathcal{S}} \frac{y_i}{\pi_i},$$

where $\mathcal{S} \subset \{1, 2, \ldots, N\}$ and $0 < \pi_i < 1$ is the inclusion probability of the ith point.

What is spatially-balanced sampling?

- A spatial sampling design determines where sample locations are placed.
- Most populations are distributed over space but many sampling designs, for example simple random sampling, do not incorporate the spatial aspect into the design.

  Natural resources often exhibit spatial trends because nearby locations interact with one another and are influenced by the same set of natural and anthropogenic factors (Stevens and Olsen, 2004).

- If nearby locations are more similar than locations further apart (a common feature), then there are statistical advantages to spreading the sample locations evenly over the population. A sample that is *evenly spread* is called a spatially balanced sample.

Spatial balance (continuous)

- Consider drawing n sample locations from a continuous resource $\Omega \subset [0,1)^2$ with $\lambda(\Omega) > 0$, where λ is the Lebesgue measure.
- Let $\pi(\boldsymbol{x}) = nf(\boldsymbol{x})$ be an inclusion density function, where $f(\boldsymbol{x}) : [0,1)^2 \to \mathbb{R}_{\geqslant 0}$ is a bounded probability density function such that

$$\int_{\Omega} f(\boldsymbol{x}) d\boldsymbol{x} = 1.$$

A sample, $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\} \subset \Omega$, is considered spatially balanced if

$$v_i = \int_{\omega_i} \pi(\boldsymbol{x}) d\boldsymbol{x} \approx 1 \quad \text{for all } i = 1, 2, \ldots, n,$$

where ω_i is the Voronoi polygon for $\boldsymbol{x}_i$

$$\omega_i = \left\{ \boldsymbol{x} \in [0,1)^2 : \|\boldsymbol{x} - \boldsymbol{x}_i\| \leqslant \|\boldsymbol{x} - \boldsymbol{x}_j\| \text{ for all } j = 1, 2, \ldots, n \right\}.$$

Spatial balance for equal probability sampling

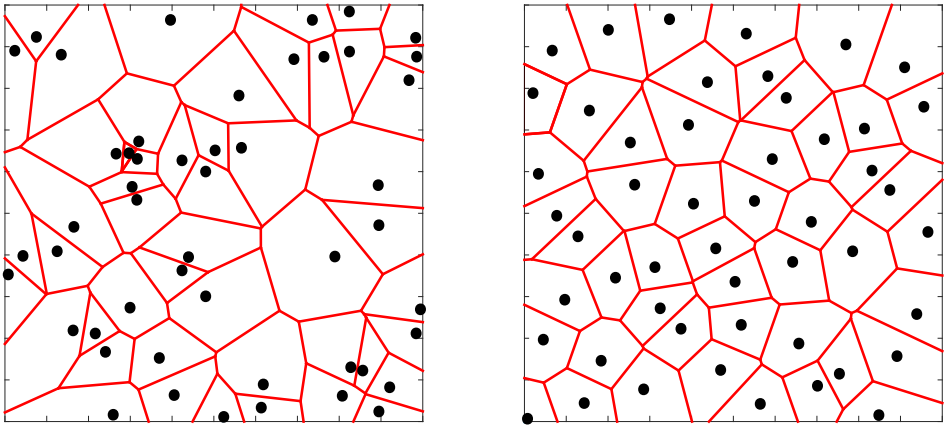


Figure: (Left) a random sample of $n = 50$ points drawn from $\Omega = [0, 1)^2$. (Right) a BAS sample of $n = 50$ points drawn from Ω. In this case, v_i is proportional to the area of ω_i (shown in red). BAS has better spatial balance than the random sample because the areas of each ω_i are more similar in size.

Spatial balance (discrete)

- Let U be a finite population of N points from $[0,1)^2$ and let $0 < \pi_i < 1$ denote the inclusion probability of $\boldsymbol{x}_i$ such that $\sum_{i=1}^{N} \pi_i = n$.

- A sample, $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\} \subset U$, is considered spatially balanced if

$$v_i = \sum_{\boldsymbol{x}_j \in \omega_i} \pi_j \approx 1 \quad \text{for all } i = 1, 2, \ldots, n,$$

where ω_i is the Voronoi set for $\boldsymbol{x}_i$

$$\omega_i = \left\{ \boldsymbol{x} \in U : \|\boldsymbol{x} - \boldsymbol{x}_i\| \leqslant \|\boldsymbol{x} - \boldsymbol{x}_j\| \text{ for all } j = 1, 2, \ldots, n \right\}.$$

Spatial balance for equal probability sampling

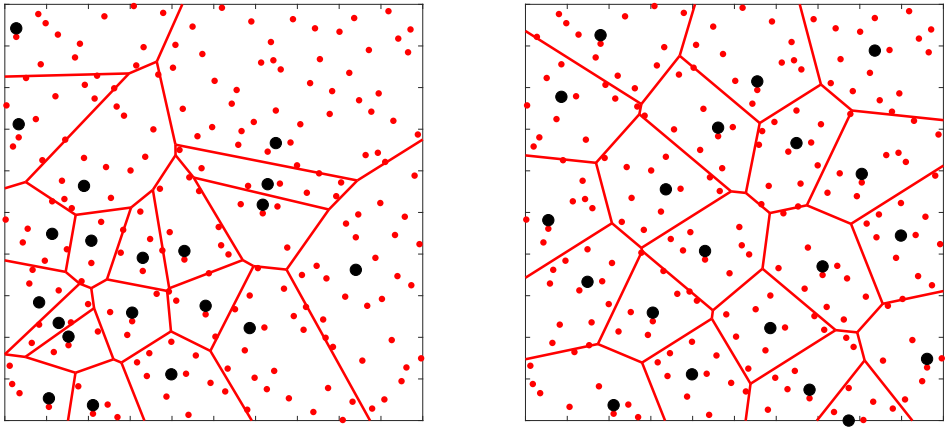


Figure: (Left) an SRS of $n = 20$ points drawn from $N = 200$ points. (Right) a HIP sample of $n = 20$ points drawn from the same 200 points. HIP has better spatial balance than SRS because the numbers of points in each ω_i are more similar.

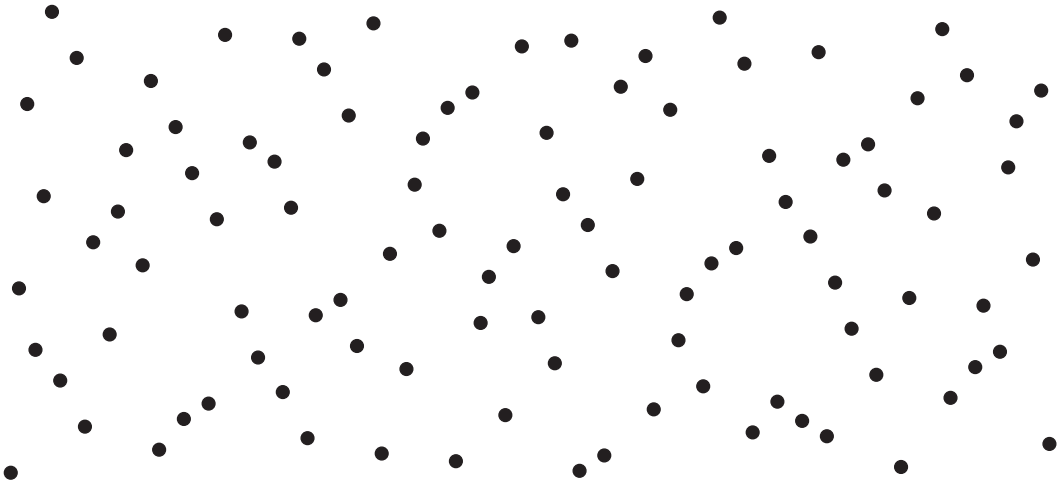
Existing Methods

- Generalized Random Tessellation Stratified (GRTS) (Stevens and Olsen 2004). The R packages `spsurvey` (Kincaid and Olsen 2015) and `SDraw` (McDonald 2016) can draw GRTS samples.

- The Local Pivotal Method (LPM) and Spatially Correlated Poisson Sampling (SCPS) (Grafström et al. 2012). The R package `BalancedSampling` (Grafström and Lisic 2016) draws LPM and SCPS samples.

- Balanced Acceptance Sampling (BAS) and Halton Iterative Partitioning (HIP) (Robertson et al. 2013,2017,2018). BAS and HIP samples can be drawn using the R package `SDraw` (McDonald 2016).

Quasi-Random Number Sequences



Psuedo-Random vs. Quasi-Random

- In practice, randomness is introduced into sampling designs using pseudo-random sequences.
- These sequences are irregular, non-repetitive and designed to mimic *true random* sequences. A sequence is considered pseudo-random if it passes a series of statistical tests including distribution type, independence of successive points, runs or combinations of digits, and so on.
- In contrast, a quasi-random sequence is not specifically designed to mimic randomness, but rather to be evenly spread over the unit box.

Quasi-Random Sequences

- A d-dimensional quasi-random sequence $H = \{\boldsymbol{x}_j\}_{j=1}^{n} \subset [0,1)^d$ is a sequence with the property that for all values of n, the sequence has low discrepancy.
- The discrepancy of H is

$$D_n(H) = \sup_{B \in \mathcal{J}} \left| \frac{A_H(B)}{n} - \lambda(B) \right|, \tag{1}$$

where λ is the Lebesgue measure, $A_H(B)$ is the number of points from H in B and $\mathcal{J}$ is the set of boxes of the form

$$\{\boldsymbol{x} \in [0,1)^d : a_i \leqslant x^{(i)} < b_i\} \quad \text{with} \quad 0 \leqslant a_i < b_i < 1. \tag{2}$$

- Loosely speaking, a sequence is considered low-discrepancy if the fraction of points in $B \in \mathcal{J}$ is proportional to $\lambda(B)$.

Quasi-Random Sequences

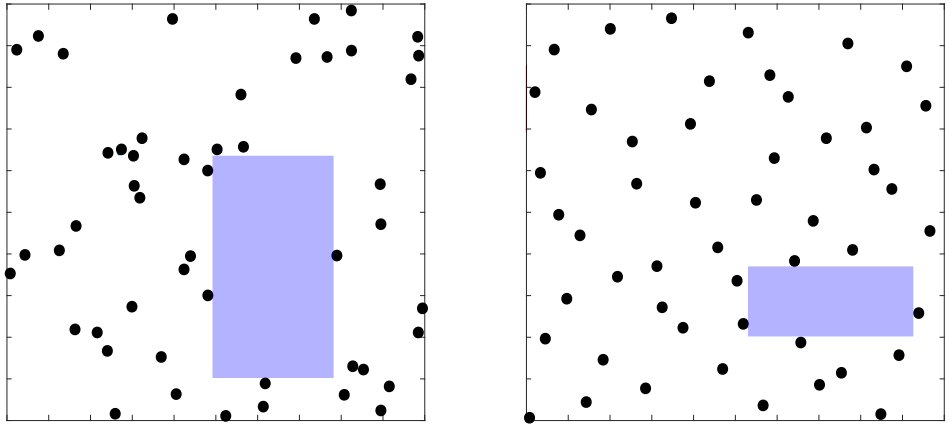


Figure: (Left) a random sample of $n = 50$ points drawn from $\Omega = [0, 1)^2$. (Right) a BAS sample of $n = 50$ points drawn from Ω. BAS is low-discrepancy, but the random sample is not.

Quasi-Random Sequences

- Quasi-random sequences have been used as a substitute for random numbers in many fields, including numerical integration, optimization and environmental sampling.

- These sequences are particularly useful because they generate evenly spread points with similar spatial properties to a regular lattice. However, unlike a regular lattice, points can be added incrementally with no clumping of points.

- There have been a number of different quasi-random sequences presented in the literature including the Halton (1960), the Sobol (1976) and the Faure (1982) sequences.

The Halton Sequence

- The ith coordinate of the jth point in the Halton sequence $\{\boldsymbol{x}_j\}_{j=1}^{\infty} \subset [0,1)^d$ is

$$x_j^{(i)} = \sum_{p=0}^{\infty} \left\{ \left\lfloor \frac{j}{b_i^p} \right\rfloor \bmod b_i \right\} \frac{1}{b_i^{p+1}},$$

  where b_i is the ith prime number and $\lfloor \cdot \rfloor$ is the floor function.

- The seventh point in the two-dimensional Halton sequence $\boldsymbol{x}_7$, for example, is

$$\begin{aligned} x_7^{(1)} &= \tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{8} + \tfrac{0}{16} + \tfrac{0}{32} + \ldots &&= \tfrac{7}{8}; \\ x_7^{(2)} &= \tfrac{1}{3} + \tfrac{2}{9} + \tfrac{0}{27} + \tfrac{0}{81} + \ldots &&= \tfrac{5}{9}; \end{aligned}$$

$$\boldsymbol{x}_7 = \left(\tfrac{7}{8}, \tfrac{5}{9}\right).$$

The Halton Sequence

- Let $B = \prod_{i=1}^{d} b_i^{J_i}$, where J_i is any non-negative integer.
- It can be shown that B consecutive points from the Halton sequence will have exactly one point in each of the Halton boxes defined by

$$\bigtimes_{i=1}^{d} \left[\frac{m_i}{b_i^{J_i}}, \frac{m_i + 1}{b_i^{J_i}} \right),$$

  where m_i is an integer satisfying $0 \leqslant m_i < b_i^{J_i}$, for all $i = 1, \ldots, d$.

- Hence, the Halton sequence is quasi-periodic (with period B) because points of the form $\boldsymbol{x}_{j+\alpha B}$ with $\alpha = 0, 1, \ldots$, are in the same box.

Halton Boxes

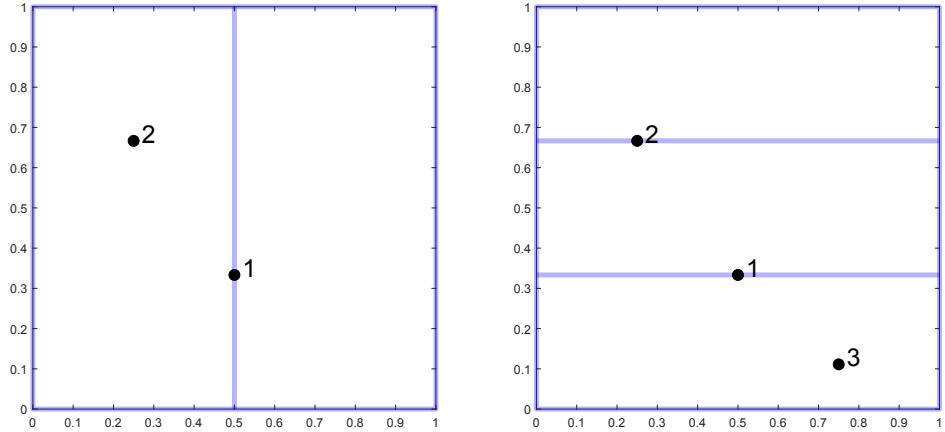


Figure: (Left) $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ with $B = 2^1 \times 3^0 = 2$. (Right) $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_3$ with $B = 2^0 \times 3^1 = 3$.

Halton Boxes

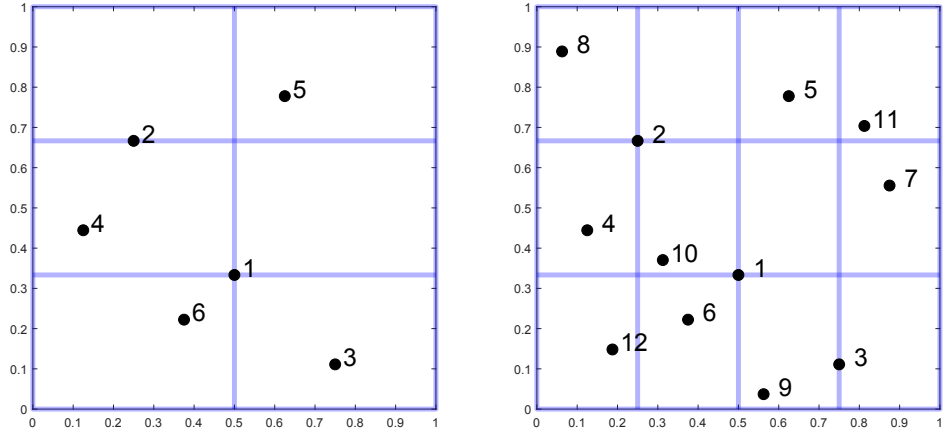


Figure: (Left) $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_6$ with $B = 2^1 \times 3^1 = 6$. (Right) $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{12}$ with $B = 2^2 \times 3^1 = 12$.

Halton Boxes

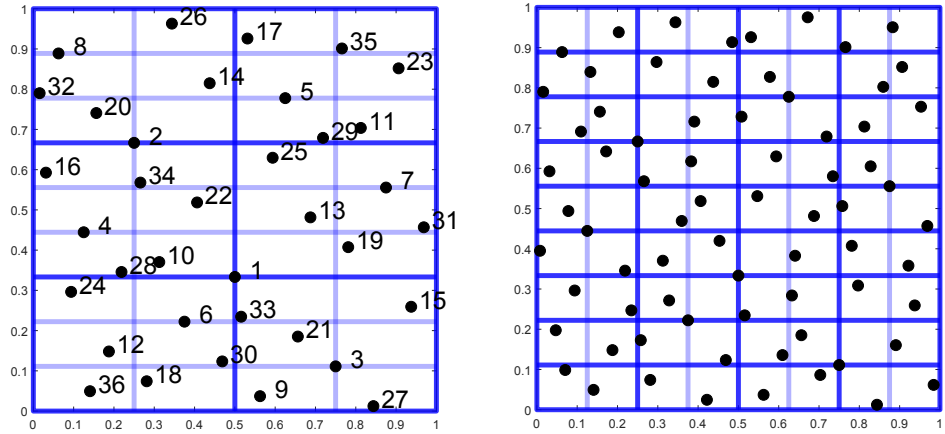
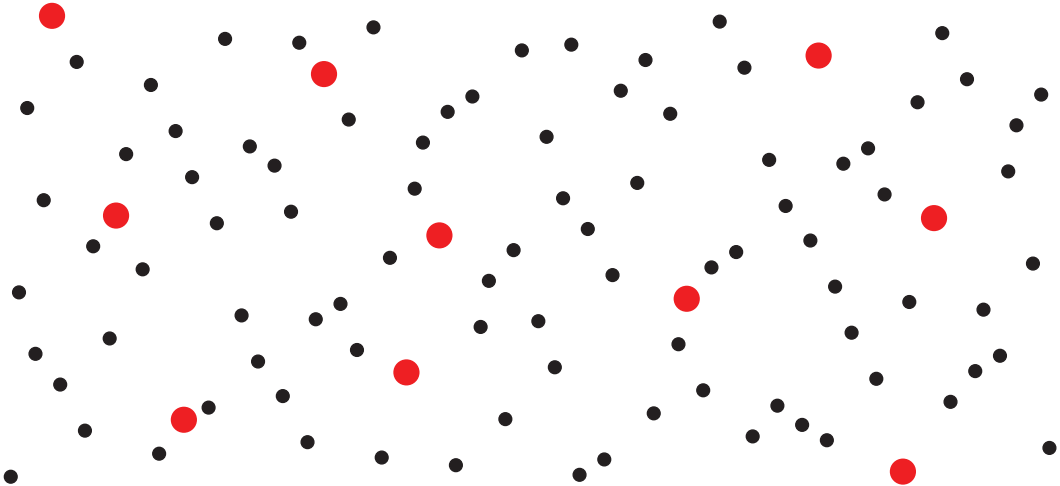


Figure: (Left) $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{36}$ with $B = 2^2 \times 3^2 = 36$. (Right) $B = 2^3 \times 3^2 = 72$.

Quasi-random spatially balanced sampling



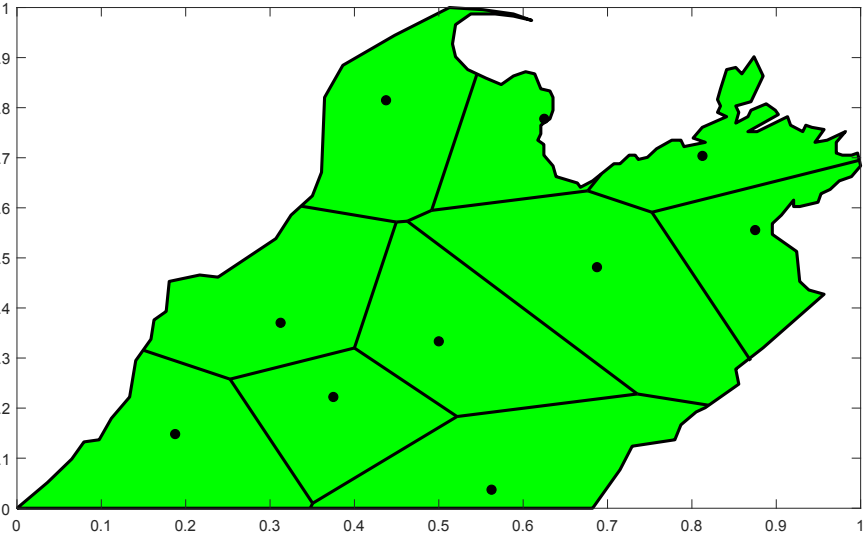
Balanced Acceptance Sampling (BAS)

- BAS is a spatially balanced sampling design that draws its sample using the random-start Halton sequence.
- The ith coordinate of the jth point in this sequence $\{\boldsymbol{x}_j\}_{j=1}^{\infty} \subset [0,1)^d$ is

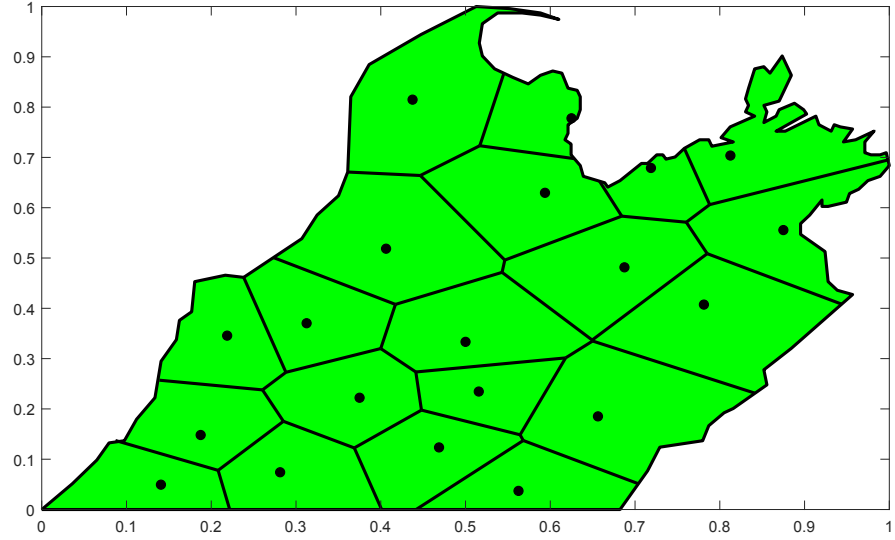
$$x_j^{(i)} = \sum_{p=0}^{\infty} \left\{ \left\lfloor \frac{u_i + j}{b_i^p} \right\rfloor \bmod b_i \right\} \frac{1}{b_i^{p+1}},$$

  where u_i is a random non-negative integer, b_i is the ith prime number and $\lfloor \cdot \rfloor$ is the floor function.
- Consider drawing n sample locations from a continuous resource $\Omega \subset [0,1]^2$ with $\lambda(\Omega) > 0$, where λ is the Lebesgue measure. An equal probability BAS sample is simply the first n points from a random-start Halton sequence that fall within Ω. However, if $\boldsymbol{x}_1 \notin \Omega$, discard the sequence and generate another.

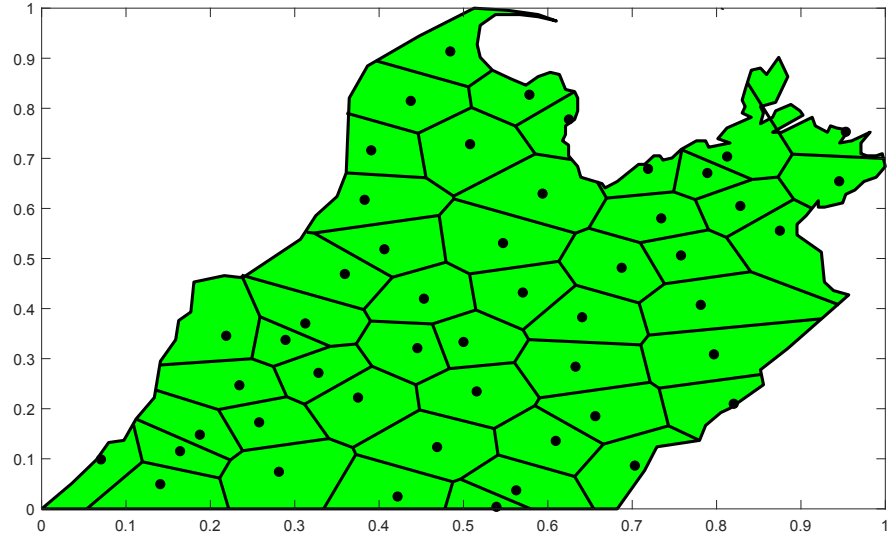
BAS ($n = 10$)



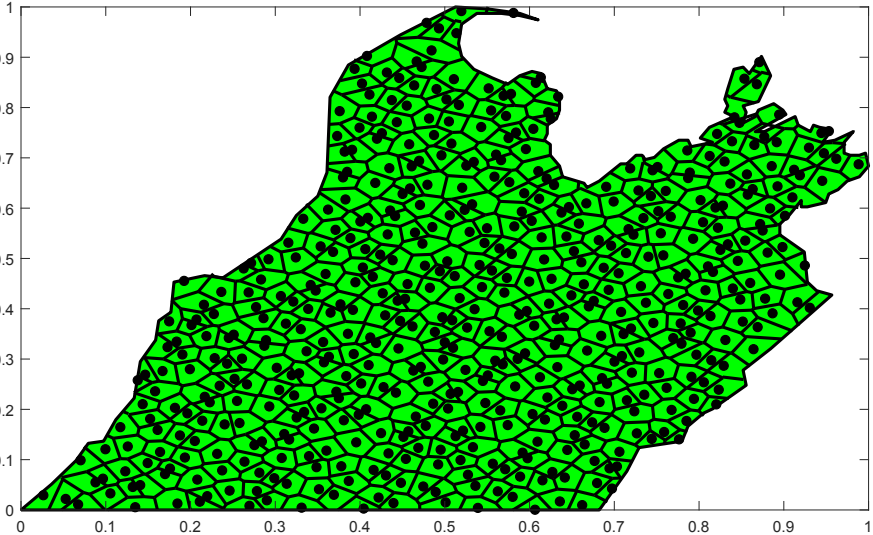
BAS ($n = 20$)



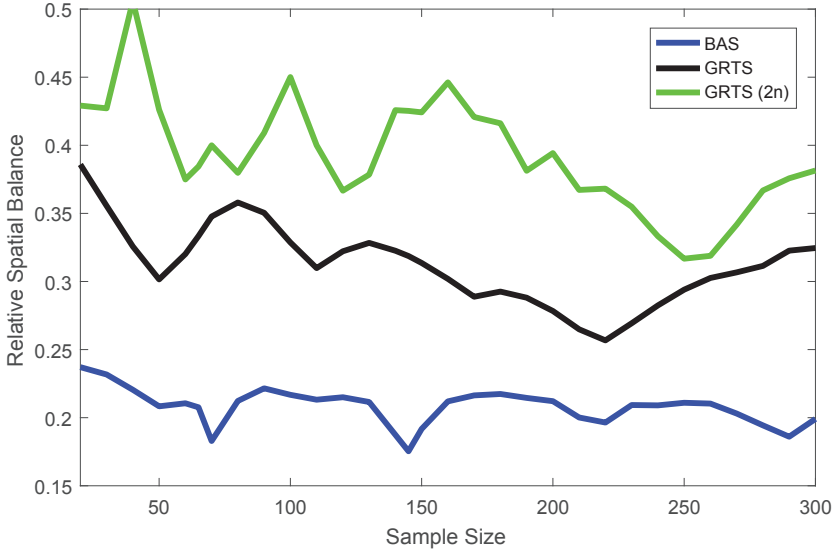
BAS ($n = 50$)



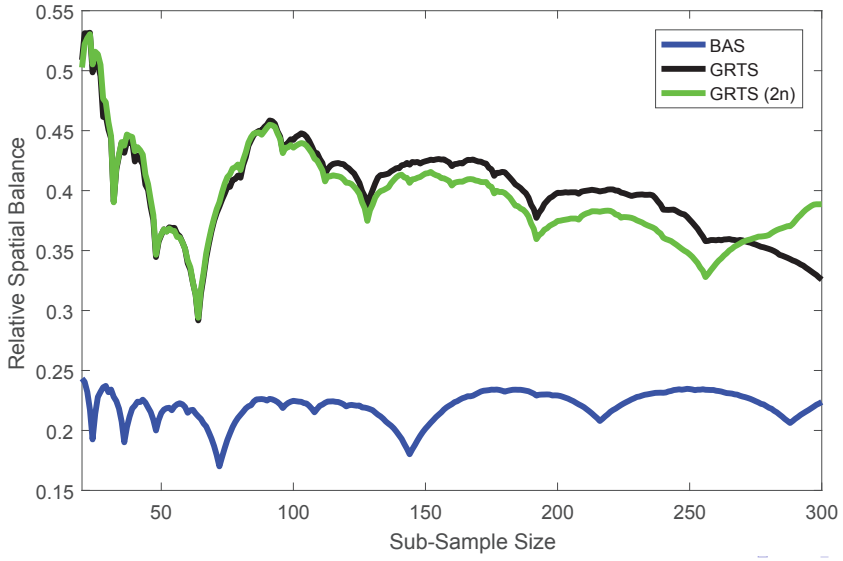
BAS ($n = 500$)



Spatial balance ($\Omega = [0,1)^2$)



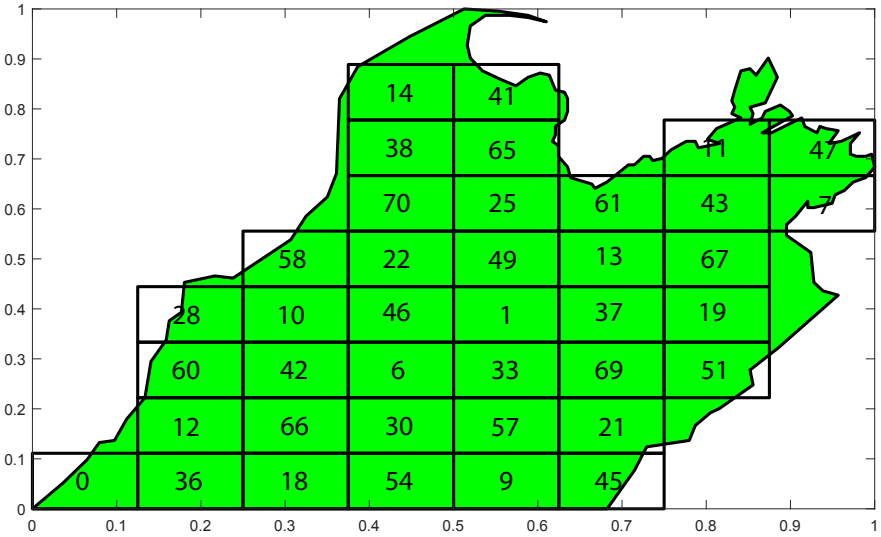
Spatial balance as points are added to the sample one-by-one ($\Omega = [0,1)^2$)



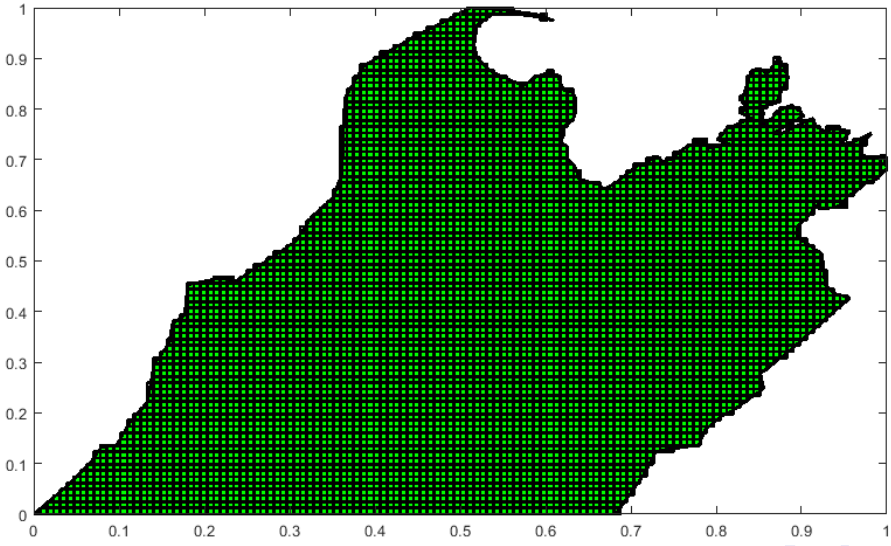
Balanced Acceptance Sampling (BAS)

- BAS is conceptually simple, computationally efficient and can be used to draw spatially balanced over-samples.
- BAS can draw samples from finite populations, but it should only be used if the resource has grid structure. Otherwise BAS can be inefficient and spatial balance can be lost.
- One useful grid structure is called a Halton frame, which is a collection of Halton boxes that intersect the resource.

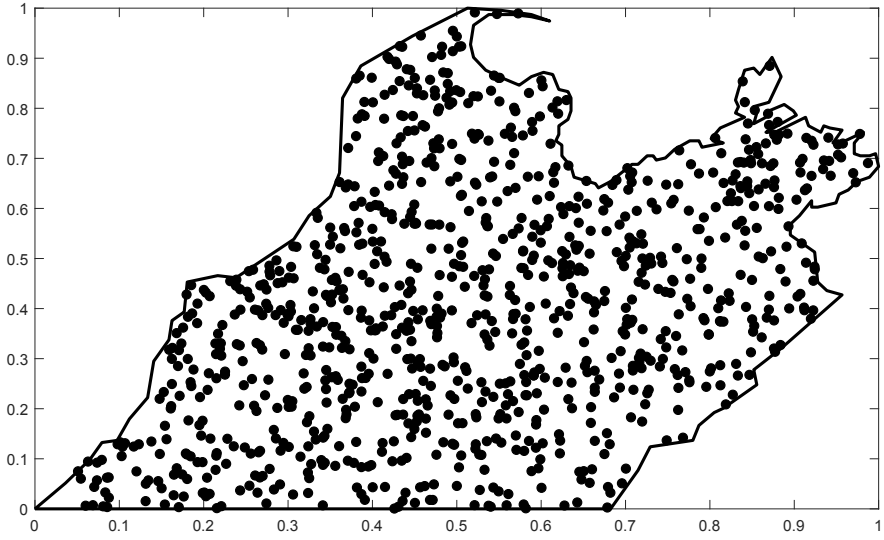
Halton Frame ($N = 39$, using $B = 2^3 \times 3^2 = 72$)



Halton Frame ($N = 5624$, using $B = 2^7 \times 3^4 = 10,368$)



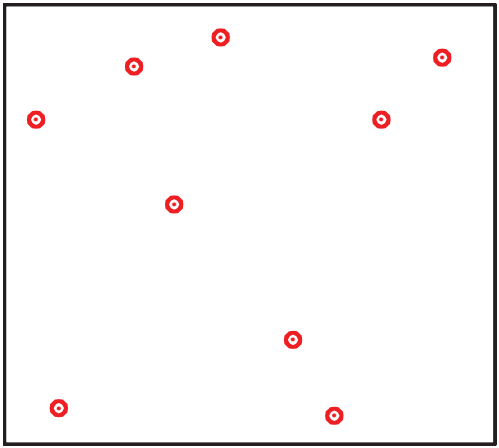
An $N = 1000$ point resource



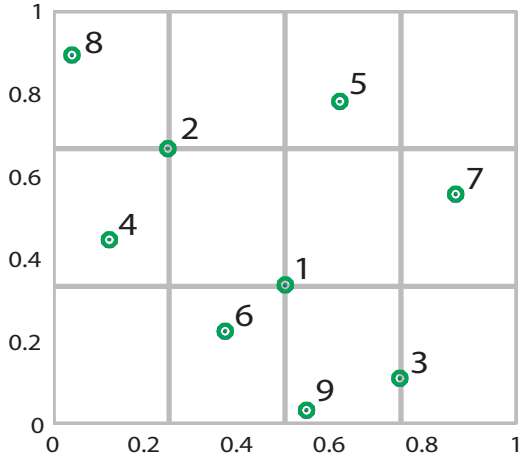
Halton Iterative Partitioning (HIP)

- Halton iterative partitioning (HIP) extends BAS to better handle point resources.
- HIP iteratively partitions a resource into $B \geqslant n$ boxes with the same nested structure as Halton boxes. These boxes are then uniquely numbered using a random-start Halton sequence of length B and the HIP sample is obtained by randomly drawing one point from each of the boxes numbered $1, 2, \ldots, n$.
- HIP is conceptually simple, computationally efficient, can be applied to continuous and point resources and achieves targeted inclusion probabilities (or density). It uses the same ordering as the Halton sequence to ensure contiguous sub-samples are spatially balanced, making it particularly useful for spatially balanced over-sampling (or a master sample) if non-target or inaccessible units are discovered.

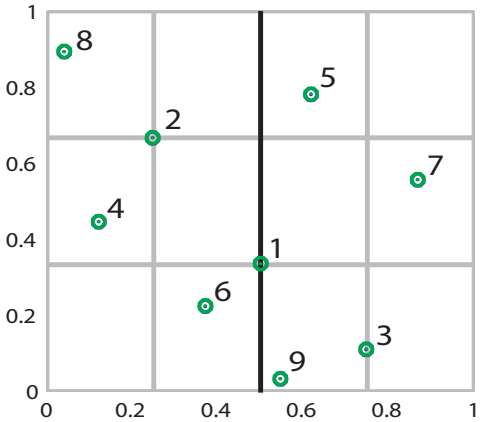
An $N = 9$ point resource

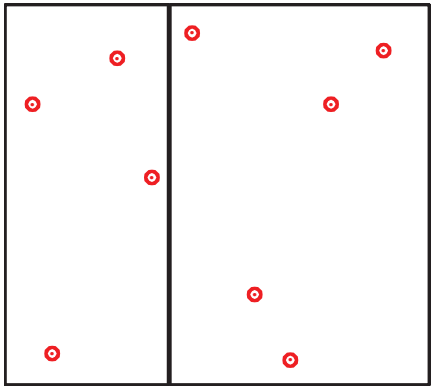


Points $x_1, \ldots, x_9$ from the Halton sequence and $B = 2^2 \times 3 = 12$ boxes

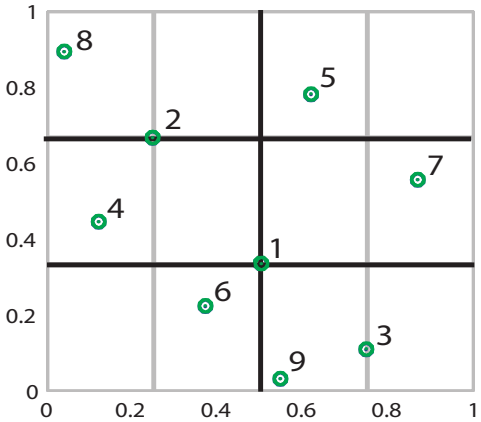


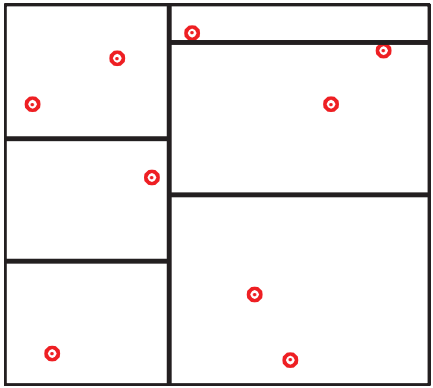
Partition with $B = 2 \times 3^0 = 2$ boxes



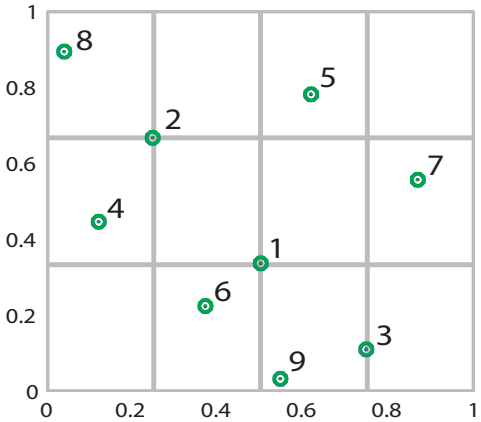


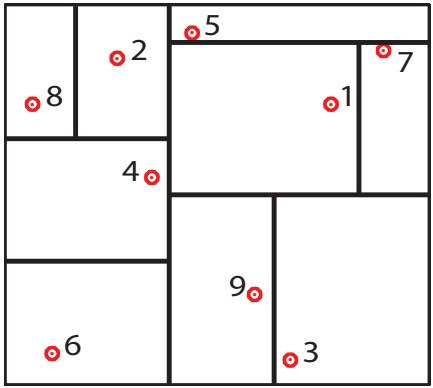
Partition with $B = 2 \times 3 = 6$ boxes



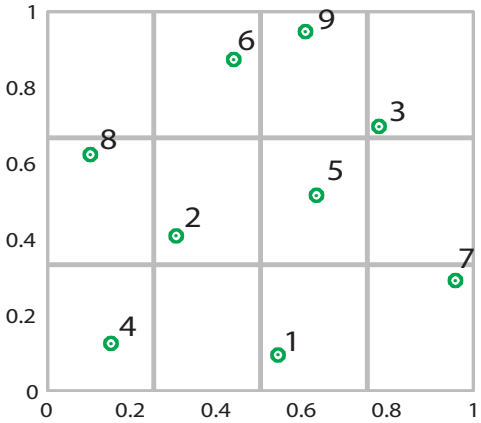


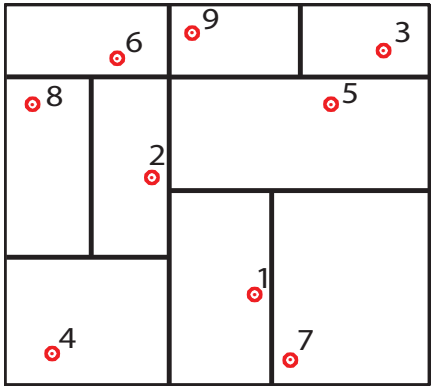
Partition with $B = 2^2 \times 3 = 12$ boxes



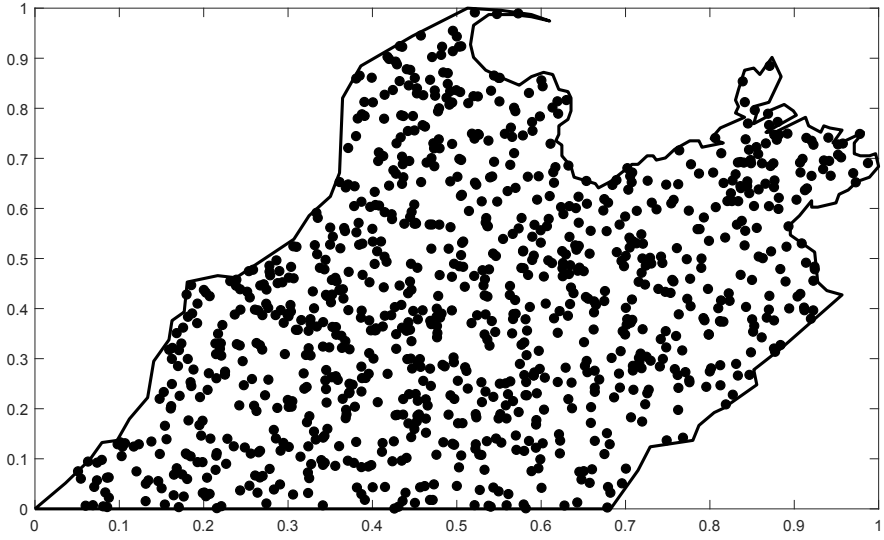


A random-start Halton sequence partition with $B = 2^2 \times 3 = 12$ boxes

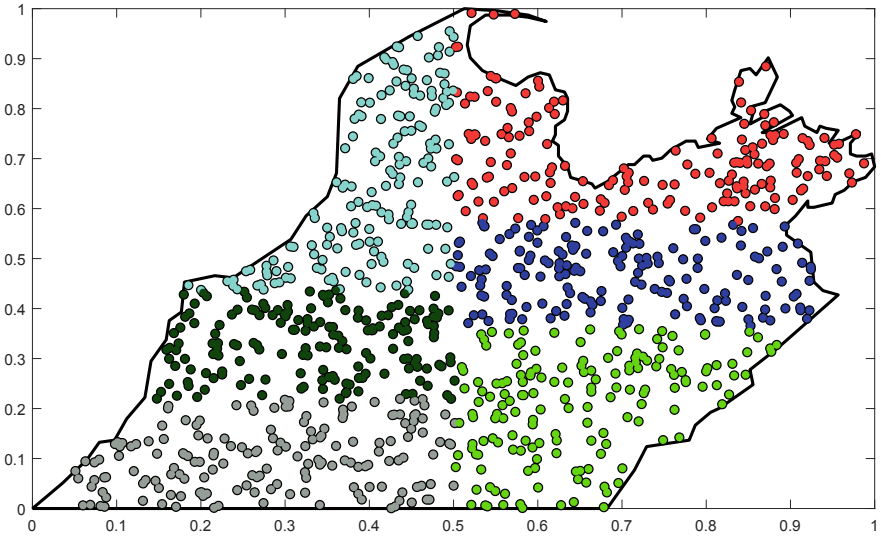




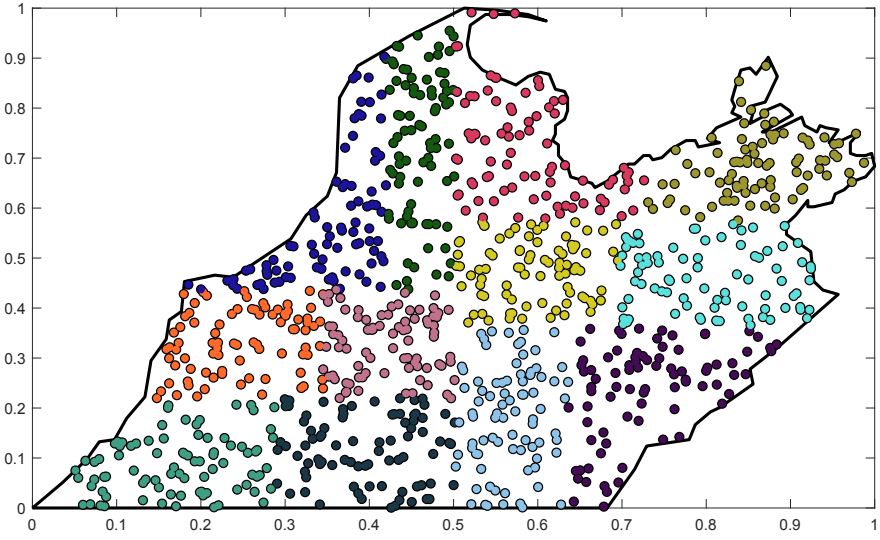
An $N = 1000$ point resource



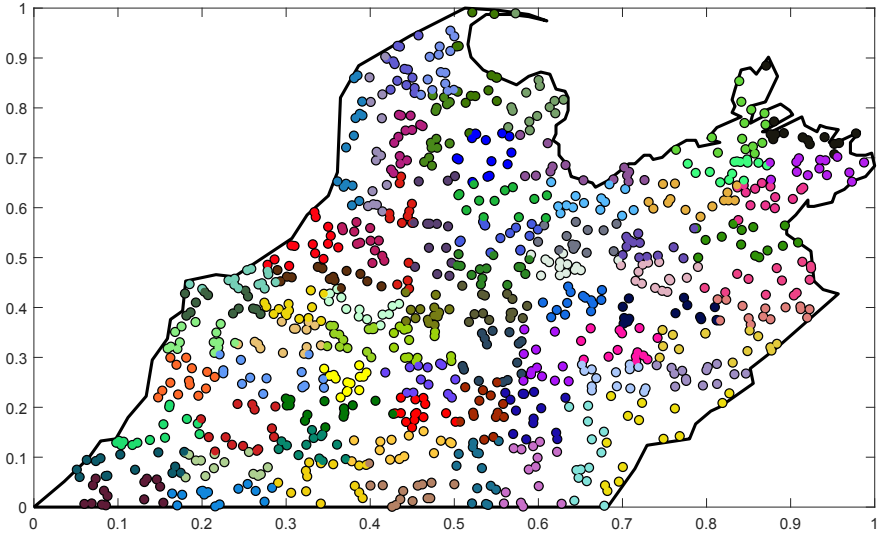
Partition with $B = 2 \times 3 = 6$ boxes



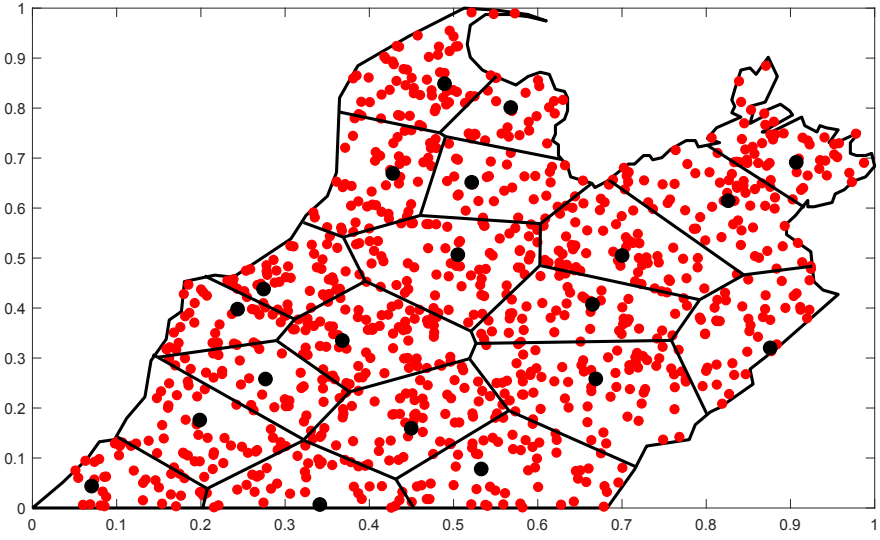
Partition with $B = 2^2 \times 3 = 12$ boxes



Partition with $B = 2^3 \times 3^2 = 72$ boxes



HIP ($n = 20$)



Permutation of box numbers for $B = 2^2 \times 3^2 = 36$ Halton boxes

	mod 36	mod 12	mod 6	mod 2
Original	$\begin{pmatrix} 8 & 26 & 17 & 35 \\ 32 & 14 & 5 & 23 \\ 20 & 2 & 29 & 11 \\ 16 & 34 & 25 & 7 \\ 4 & 22 & 13 & 31 \\ 28 & 10 & 1 & 19 \\ 24 & 6 & 33 & 15 \\ 12 & 30 & 21 & 3 \\ 0 & 18 & 9 & 27 \end{pmatrix}$	$\begin{pmatrix} 8 & 2 & 5 & 11 \\ 8 & 2 & 5 & 11 \\ 8 & 2 & 5 & 11 \\ 4 & 10 & 1 & 7 \\ 4 & 10 & 1 & 7 \\ 4 & 10 & 1 & 7 \\ 0 & 6 & 9 & 3 \\ 0 & 6 & 9 & 3 \\ 0 & 6 & 9 & 3 \end{pmatrix}$	$\begin{pmatrix} 2 & 2 & 5 & 5 \\ 2 & 2 & 5 & 5 \\ 2 & 2 & 5 & 5 \\ 4 & 4 & 1 & 1 \\ 4 & 4 & 1 & 1 \\ 4 & 4 & 1 & 1 \\ 0 & 0 & 3 & 3 \\ 0 & 0 & 3 & 3 \\ 0 & 0 & 3 & 3 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$
Permutation	$\begin{pmatrix} 13 & 31 & 22 & 4 \\ 1 & 19 & 10 & 28 \\ 25 & 7 & 34 & 16 \\ 17 & 35 & 26 & 8 \\ 29 & 11 & 2 & 20 \\ 5 & 23 & 14 & 32 \\ 33 & 15 & 6 & 24 \\ 21 & 3 & 30 & 12 \\ 9 & 27 & 18 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 7 & 10 & 4 \\ 1 & 7 & 10 & 4 \\ 1 & 7 & 10 & 4 \\ 5 & 11 & 2 & 8 \\ 5 & 11 & 2 & 8 \\ 5 & 11 & 2 & 8 \\ 9 & 3 & 6 & 0 \\ 9 & 3 & 6 & 0 \\ 9 & 3 & 6 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 4 & 4 \\ 1 & 1 & 4 & 4 \\ 1 & 1 & 4 & 4 \\ 5 & 5 & 2 & 2 \\ 5 & 5 & 2 & 2 \\ 5 & 5 & 2 & 2 \\ 3 & 3 & 0 & 0 \\ 3 & 3 & 0 & 0 \\ 3 & 3 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$

Estimation

- The Horvitz-Thompson (HT) estimator of the population total τ is

$$\widehat{\tau} = \sum_{i \in \mathcal{S}} \frac{y_i}{\pi_i},$$

where $\mathcal{S} \subset \{1, 2, \ldots, N\}$ and π_i is the inclusion probability of the ith point.

- The variance of the HT estimator for a fixed sample size can be written as

$$V(\widehat{\tau}) = -\frac{1}{2} \sum_{i,j} (\pi_{ij} - \pi_i \pi_j) \left(\frac{y_i}{\pi_i} - \frac{y_j}{\pi_j} \right)^2,$$

and can be estimated from a sample using the Sen-Yates-Grundy estimator

$$\widehat{V}(\widehat{\tau}) = -\frac{1}{2} \sum_{i,j \in \mathcal{S}} \frac{\pi_{ij} - \pi_i \pi_j}{\pi_{ij}} \left(\frac{y_i}{\pi_i} - \frac{y_j}{\pi_j} \right)^2,$$

where π_{ij} is the second order inclusion probability.

Estimation

- The local mean variance estimator (Stevens and Olsen 2003) is

$$\widehat{\mathrm{V}}_{\mathrm{NBH}}(\widehat{\tau}) = \sum_{i \in \mathcal{S}} \sum_{j \in D_i} w_{ij} \left(\frac{y_j}{\pi_j} - \widehat{\tau}_{D_i} \right)^2, \tag{3}$$

where D_i is a neighbourhood containing at least four nearest neighbours to the ith point, $\widehat{\tau}_{D_i}$ is an estimate of the population total on D_i and w_{ij} are weights.

- Another variance estimator (Grafström and Schelin 2014) is,

$$\widehat{\mathrm{V}}_{\mathrm{G}}(\widehat{\tau}) = \frac{1}{2} \sum_{i \in \mathcal{S}} \left(\frac{y_i}{\pi_i} - \frac{y_{j_i}}{\pi_{j_i}} \right)^2, \tag{4}$$

where $j_i \in \mathcal{S}$ is the index of the nearest neighbour in the sample to the ith point.

Estimation (N = 10,000)

Table: The reported values are averages using 1000 different samples, where V_{SIM} is the empirical variance estimator. Exact values are shown for SRS, V_{SRS}.

Pop	n	SRS	GRTS		GRTS ($2n$)		HIP		
		V_{SRS}	V_{SIM}	$\widehat{V}_{NBH}$	V_{SIM}	$\widehat{V}_{NBH}$	V_{SIM}	$\widehat{V}_{NBH}$	$\widehat{V}_{G}$
1	20	0.1044	0.0210	0.0282	0.0247	0.0279	**0.0132**	0.0298	0.0160
	50	0.0416	0.0041	0.0053	0.0094	0.0051	**0.0023**	0.0055	0.0026
	100	0.0207	0.0012	0.0014	0.0041	0.0014	**0.0006**	0.0015	0.0007
	150	0.0137	0.0006	0.0006	0.0019	0.0006	**0.0002**	0.0007	0.0003
	200	0.0103	0.0004	0.0004	0.0008	0.0003	**0.0002**	0.0004	0.0002
2	20	0.1812	0.0801	0.1164	0.0875	0.1122	**0.0699**	0.1162	0.1110
	50	0.0722	0.0171	0.0321	0.0285	0.0303	**0.0131**	0.0331	0.0218
	100	0.0359	0.0071	0.0103	0.0121	0.0100	**0.0041**	0.0108	0.0057
	150	0.0238	0.0036	0.0051	0.0069	0.0049	**0.0019**	0.0053	0.0026
	200	0.0178	0.0018	0.0031	0.0036	0.0029	**0.0010**	0.0031	0.0015
3	20	74.614	44.805	45.405	43.332	45.491	**31.667**	48.464	45.947
	50	29.756	9.016	13.304	12.275	12.913	**7.937**	13.590	9.843
	100	14.803	2.873	4.431	5.480	4.316	**1.686**	4.660	2.759
	150	9.819	1.448	2.215	3.096	2.099	**0.990**	2.316	1.262
	200	7.327	0.811	1.348	1.562	1.278	**0.671**	1.368	0.714

Concluding Remarks

- Spatially balanced sampling designs are useful if nearby points are expected to have similar response values and a variety of designs have been proposed.
- BAS and HIP are spatially balanced designs that utilise the Halton sequence.
- The potential advantages of these designs over other spatially balanced designs include being conceptually simple, computationally efficient, being able to adjust sample sizes dynamically and draw spatially balanced over-samples (or master samples).
- Spatially balanced over-sampling is particularly useful for sampling natural resources because imperfect sampling frames and accessibility problems can result in fewer units being observed than planned. Although the over-sampling strategy achieves the desired sample size and is popular with field researchers, it will not eliminate the non-response or the bias of an inference.

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